

Control of quantum transmission is trap free

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Abstract

We consider manipulation of the transmission coefficient for a quantum particle moving in one dimension where the shape of the potential is taken as the control. We show that the control landscape—the transmission as a functional of the potential—has no traps, i.e., any maxima correspond to full transmission.

Keywords: Quantum control, transmission coefficient, control landscape

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1 Introduction

Control of atomic and molecular scale systems obeying quantum equations of motion is an important branch of modern science. Applications range from selective excitation of atomic or molecular states to laser control of chemical reactions and high harmonic generation [1, 2, 3, 4, 5, 6, 7]. One of the major questions in quantum control theory is whether for a given objective the control landscape has traps, that is, local maxima with values less than the global maximum [8, 9]. Much effort has been directed towards the study of control landscapes of n -level systems. Despite this effort, the proof of trap free behavior has been obtained so far only for two-level systems [10]. The case of systems with an infinite dimensional Hilbert space has not been treated at all.

Here we consider control of transmission of a quantum particle moving through a potential barrier where the shape of the potential is used as a control parameter. This is relevant, for example, to control of tunneling [11, 12, 13]. We show that the landscape of the transmission coefficient of a quantum particle as a functional of the potential is trap free, i.e., any maxima correspond to full transmission.

2 Formulation

Consider a particle of a fixed energy E scattering on a barrier of potential $V(x)$ which is assumed to have compact support ($V(x) = 0$ when $|x| > a$ for some a). The particle wavefunction satisfies the time-independent Schrödinger equation

$$H_V \Psi(x) = E \Psi(x) \tag{1}$$

where

$$H_V = -\frac{d^2}{dx^2} + V(x).$$

We take the mass $m = 1/2$ and $\hbar = 1$.

The second-order differential equation (1) has two independent solutions. We are free to choose linear combinations of the solutions that behave as [14]

$$\Psi_1^0(x) = \begin{cases} e^{ik_E x} + A_E e^{-ik_E x}, & x < -a \\ B_E e^{ik_E x}, & x > a \end{cases} \quad (2a)$$

$$\Psi_2^0(x) = \begin{cases} D_E e^{-ik_E x}, & x < -a \\ e^{-ik_E x} + C_E e^{ik_E x}, & x > a \end{cases}. \quad (2b)$$

Here $k_E = \sqrt{E}$. The solution Ψ_1^0 describes the particle incident on the barrier from the left. The particle is partially reflected and partially transmitted through the barrier. Thus the wavefunction on the left, far away from the barrier, is a sum of the incoming and reflected waves, $\Psi_1^0(x) = e^{ik_E x} + A_E e^{-ik_E x}$ ($x \rightarrow -\infty$), whereas on the right of the barrier the wavefunction is an outgoing wave, $\Psi_1^0(x) = B_E e^{ik_E x}$ ($x \rightarrow +\infty$). The coefficients A_E and B_E determine the probabilities of reflection and transmission, respectively. The transmission coefficient is defined as the amplitude of the transmitted wave, $T_E[V] = |B_E|^2$, and describes the probability of transmission through the barrier. Similarly, the solution Ψ_2^0 describes the particle incident on the barrier from the right, which is partially reflected back to the right and partially transmitted to the left [15].

2.1 Kinematic control landscape

The general solution of Eq. (1) as $x \rightarrow -\infty$ is a sum of incoming and reflected waves $\Psi(x) = A'e^{ik_E x} + Ae^{-ik_E x}$ and as $x \rightarrow +\infty$ is $\Psi(x) = Be^{ik_E x} + B'e^{-ik_E x}$. The coefficients B and B' are linearly related to the coefficients A' and A by a 2×2 matrix M which is called the *monodromy operator*:

$$\begin{pmatrix} B \\ B' \end{pmatrix} = M \begin{pmatrix} A' \\ A \end{pmatrix}.$$

The monodromy operator is an element of the *special (1, 1) unitary group* $SU(1, 1)$ also called the *real symplectic group of second order* $Sp(1, \mathbb{R})$ [16]. Any element of this group can be represented as

$$M = \begin{pmatrix} \sqrt{1 + |z|^2}e^{i\phi} & z \\ \bar{z} & \sqrt{1 + |z|^2}e^{-i\phi} \end{pmatrix}$$

where $z \in \mathbb{C}$ and $\phi \in [0, 2\pi)$.

Consider a wave incident on the potential from left infinity. Then $A' = 1$, $B' = 0$ and the equality

$$\begin{pmatrix} B \\ 0 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} 1 \\ A \end{pmatrix}$$

implies $A = -M_{21}/M_{22}$ and $B = 1/M_{22}$. This gives for the transmission coefficient (as a

function of M) the *kinematic* expression

$$T(M) = |B|^2 = \frac{1}{|M_{22}|^2} = \frac{1}{1 + |z|^2} \quad (3)$$

Theorem 1 *The only extrema of $T(M)$ over $M \in SU(1, 1)$ are global maxima. These occur at $z = 0$, where*

$$M = \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix}, \quad \phi \in [0, 2\pi).$$

Proof. The theorem follows from eq. (3) and the domain of z .

Theorem 1 shows that the control landscape of the transmission coefficient has no kinematic traps and that its only kinematic extrema are global maxima corresponding to full transmission.

2.2 Dynamic control landscape

What is of ultimate interest is to know if the *dynamic* landscape of the transmission coefficient has traps, i.e. whether the transmission coefficient as a functional of the potential $V(x)$, has any local maxima or only a global maximum for full transmission. In this section we prove that there are no traps, i.e. all extrema of the transmission coefficient $T_E[V]$ as a functional of the potential are only global maxima.

We will use the known result that for sufficiently smooth functions $f(E)$ and $S(E)$

$$\int_{\mathbb{R}} \frac{e^{ixS(E_f)} f(E_f)}{E_f - E_i - i0} dE_f = i\pi[1 + \operatorname{sgn} S'(E_i)]f(E_i)e^{ixS(E_i)} + O(x^{-\infty}) \quad (4)$$

provided $S'(E_0) \neq 0$ [17, 18].

Theorem 2 *The only extrema of the objective $J[V] = T_E[V]$ are global maxima.*

Proof. Let $\Psi_{\alpha, E_i}^0(x)$ ($\alpha = 1, 2$) be two eigenfunctions of H_V with energy E . Consider a small variation of the potential $V(x) \rightarrow V(x) + \delta v(x)$. The modification of the eigenfunction with energy E due to the variation of the potential can be computed using perturbation theory for continuous spectrum as follows (we omit a sum over the discrete spectrum since the transmission coefficient depends only on the behavior of the wave function at infinity, where wavefunctions corresponding to the discrete spectrum vanish)

$$\Psi_{1, E_i} = \Psi_{1, E_i}^0 + \underbrace{\int \frac{\langle \Psi_{1, E_f}^0, \delta v \Psi_{1, E_i}^0 \rangle}{E_i - E_f + i0} \Psi_{1, E_f}^0 dE_f}_{\delta \Psi_1(x)} + \underbrace{\int \frac{\langle \Psi_{2, E_f}^0, \delta v \Psi_{1, E_i}^0 \rangle}{E_i - E_f + i0} \Psi_{2, E_f}^0 dE_f}_{\delta \Psi_2(x)} + o(\|\delta v\|) \quad (5)$$

Here $\langle \Psi_{\alpha, E_f}^0, \delta v \Psi_{1, E_i}^0 \rangle = \int_{\mathbb{R}} \overline{\Psi_{\alpha, E_f}^0}(x) \delta v(x) \Psi_{1, E_i}^0(x) dx$ for $\alpha = 1, 2$.

The transmission coefficient at energy E_i for the modified potential $V + \delta v$ up to linear order in δv can be computed as

$$\begin{aligned} T_{E_i}[V + \delta v] &= \lim_{x \rightarrow +\infty} |\Psi_{1, E_i}(x)|^2 \\ &= \lim_{x \rightarrow +\infty} \left\{ |\Psi_{1, E_i}^0(x)|^2 + 2\Re \left[\overline{\Psi_{1, E_i}^0}(x) \left(\delta \Psi_1(x) + \delta \Psi_2(x) \right) \right] \right\} + o(\|\delta v\|) \\ &= T_{E_i}[V] + \delta J(V) + o(\|\delta v\|) \end{aligned}$$

By eqs. (2a), (4), and (5)

$$\begin{aligned}
\lim_{x \rightarrow +\infty} 2\Re[\bar{\Psi}_{1,E_i}^0(x)\delta\Psi_1(x)] &= -2\Re \lim_{x \rightarrow +\infty} \int \frac{\langle \Psi_{1,E_f}^0, \delta v \Psi_{1,E_i}^0 \rangle}{E_f - E_i - i0} B_{E_i}^* B_{E_f} e^{i(k_{E_f} - k_{E_i})x} \\
&= -4\pi \Im[\langle \Psi_{1,E_i}^0, \delta v \Psi_{1,E_i}^0 \rangle |B_{E_i}|^2] = 0
\end{aligned}$$

Here the second equality follows from (4) with $S(E_f) = k_{E_f} - k_{E_i}$ which gives $\text{sgn } S'(E_f)|_{E_f=E_i} = 1$, and the last equality follows from the fact that diagonal matrix elements of δv are real.

Similarly,

$$\begin{aligned}
&\lim_{x \rightarrow +\infty} 2\Re[\bar{\Psi}_{1,E_i}^0(x)\delta\Psi_2(x)] \\
&= -2\Re \lim_{x \rightarrow +\infty} \int \frac{\langle \Psi_{2,E_f}^0, \delta v \Psi_{1,E_i}^0 \rangle}{E_f - E_i - i0} B_{E_i}^* e^{-ik_{E_i}x} [e^{-ik_{E_f}x} + C_{E_f} e^{ik_{E_f}x}] dE_f \\
&= -2\Re \lim_{x \rightarrow +\infty} \int \frac{\langle \Psi_{2,E_f}^0, \delta v \Psi_{1,E_i}^0 \rangle}{E_f - E_i - i0} B_{E_i}^* [e^{-i(k_{E_f} + k_{E_i})x} + C_{E_f} e^{i(k_{E_f} - k_{E_i})x}] dE_f
\end{aligned}$$

The term with $e^{-i(k_{E_f} + k_{E_i})x}$ in the square brackets gives zero contribution in the limit since for this term $S(E_f) = -k_{E_f} - k_{E_i}$ gives $\text{sgn } S'(E_f) = -1$ and the integral is $O(x^{-\infty})$ according to (4). The contribution of the term with $e^{i(k_{E_f} - k_{E_i})x}$ in the square brackets can be computed using equality (4) as follows:

$$\begin{aligned}
-2 \lim_{x \rightarrow +\infty} \Re \int \frac{\langle \Psi_{2,E_f}^0, \delta v \Psi_{1,E_i}^0 \rangle}{E_f - E_i - i0} B_{E_i}^* C_{E_f} e^{i(k_{E_f} - k_{E_i})x} dE_f &= -4\pi \Re [i \langle \Psi_{2,E_i}^0, \delta v \Psi_{1,E_i}^0 \rangle B_{E_i}^* C_{E_i}] \\
&= -4\pi |B_{E_i}|^2 \Im \left[\langle \Psi_{2,E_i}^0, \delta v \Psi_{1,E_i}^0 \rangle \frac{A_{E_i}^*}{B_{E_i}^*} \right] \\
&= -4\pi T_{E_i}[V] \Im \left[\langle \Psi_{2,E_i}^0, \delta v \Psi_{1,E_i}^0 \rangle \frac{A_{E_i}^*}{B_{E_i}^*} \right] \\
&= \delta J(V)
\end{aligned}$$

Here we have used the fact for any E

$$C(E) = -\frac{B(E)A^*(E)}{B^*(E)}$$

(see Eqs. (7.84) and (7.86) in [5]).

A critical potential $V(x)$ should satisfy $\delta J(V) = 0$ for any δv . Since for any E $B(E) \neq 0$ and $T_E[V] \neq 0$, this is possible only if $A(E_i) = 0$. That corresponds to $T_{E_i}[V] = 1$, i.e., any critical potential leads to a global maximum of the transmission coefficient. This concludes the proof of the theorem.

3 Comparison with the landscape for coherent control by lasers

Quantum control landscapes for n -level systems controlled by lasers or electro-magnetic fields have been extensively studied in recent years. In this section, we put our findings about the landscape for control of transmission in the context of what is known about the landscape for coherent control of n -level systems by lasers. We assume that the n -level system interacts only with the laser and is isolated from other environments, i.e., is a closed quantum system.

The evolution equation for a system controlled by a laser field $\varepsilon(t)$ is the Schrödinger equation

$$i\frac{dU_t^\varepsilon}{dt} = (H_0 + \varepsilon(t)V)U_t^\varepsilon, \quad U_0^\varepsilon = \mathbb{I}$$

Here H_0 and V are the free and interaction Hamiltonians, respectively. The solution of this equation is a unitary matrix, $U_T^\varepsilon \in U(n)$. The overall phase of the unitary evolution operator

is physically meaningless, so that U and $e^{i\phi}U$ describe the same physics. Thus the space of kinematic controls for laser control is the special unitary group $SU(n)$, instead of the special $(1, 1)$ unitary group $SU(1, 1)$ for control of the transmission coefficient. The objective that corresponds to the transmission coefficient is the probability of transition from some initial state ψ_i to some final state ψ_f , $J(U_T^\varepsilon) = |\langle \psi_f | U_T^\varepsilon | \psi_i \rangle|^2$.

The kinematic landscape for the transition probability $J(U)$ (considered as a function of $U \in SU(n)$) is trap-free [8]. However, this result does not imply the absence of traps for the corresponding dynamic landscape $J(U_T^\varepsilon)$ (considered as a functional of ε) due to the existence of non-regular controls (i.e. controls where the rank of the Jacobian $\delta U_T / \delta \varepsilon(t)$ is not maximal). To see this, consider the chain rule

$$\frac{\delta J(\varepsilon)}{\delta \varepsilon(t)} = \frac{\delta J(U)}{\delta U} \Big|_{U=U_T^\varepsilon} \frac{\delta U_T^\varepsilon}{\delta \varepsilon(t)}.$$

The absence of traps for $J(U)$ implies the absence of traps for $J(\varepsilon)$ only if the Jacobian $\delta U_T^\varepsilon / \delta \varepsilon(t)$ has full rank, i.e. has no zero eigenvalues. The analogous full rank criterion for control of the transmission coefficient is that rank of the Jacobian $\delta M_V / \delta V(x)$ is maximal, where M_V is the monodromy operator for potential $V(x)$.

The only rigorous proof of the absence of dynamical traps for coherent laser control is for $n = 2$ [10]. Interestingly, the dimension of the corresponding kinematic control space $SU(2)$ is the same as the dimension of the kinematic control space $SU(1, 1)$ for control of transmission. While the resulting conclusion of trap-free dynamics is the same for these two cases, the proofs are fundamentally different.

We summarize the comparison of landscape-related notions for laser control and for

	Coherent control by laser	Control by potential
Dynamic control	Laser pulse $\varepsilon(t)$	Potential $V(x)$
Kinematic control	$U \in SU(n)$	$M \in SU(1, 1)$
Objective	$J(U) = \langle \psi_f U \psi_i \rangle ^2$	$J(M) = \frac{1}{ M_{22} ^2}$
Kinematic landscape	No traps, $\max J = 1, \min J = 0$	No traps, $\max J = 1, \inf J = 0$
Full rank criterion	Jacobian $\delta U_T^\varepsilon / \delta \varepsilon(t)$ has maximal rank	Jacobian $\delta M_V / \delta V(x)$ has maximal rank
Dynamic landscape	Generally unknown. Trap-free for $n = 2$.	Trap-free.

Table 1: Comparison of landscape-related notions for coherent control by lasers and control by potential.

control of transmission in Table 1.

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